【Grant-in-Aid for Transformative Research Areas（A）】

Integrated Science of Synthesis by Chemical Structure Reprogramming

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Project Information	Project Number : 24A202　Project Period (FY) : 2024-2028 Keywords : Chemical Synthesis, Chemical Structure Editing, Catalysis, Reaction Chemistry

Purpose and Background of the Research

●Outline of the Research

In the evolving landscape of future societies, materials must not only offer advanced functionalities but also prioritize environmental sustainability and recyclability. As materials grow increasingly intricate to meet these demands, the lack of efficient methods for their rapid synthesis remains a significant challenge hindering material innovation.

Our research introduces **Structural Re-Programming (SReP)** as a groundbreaking approach to address this bottleneck. SReP offers a versatile methodology to modify skeletal structures on demand, enabling swift construction of diverse structural frameworks. In the traditional synthesis, even a minor editing to molecular skeleton often requires repeated reactions from starting materials (LEGO-like synthesis). In contrast, SReP streamlines this multi-step process by allowing substitutions, insertions, or deletions of atom(s) within the established structure. Furthermore, SReP can grant access to structures that are currently inaccessible.

Figure 1. Goals of the research

While current chemical synthesis faces inefficiencies, particularly in editing skeletal structures, our interdisciplinary approach aims to bridge gaps across organic chemistry, inorganic chemistry, polymer chemistry, coordination chemistry, supramolecular chemistry, and biomolecular chemistry. By synergizing these fields under the umbrella of 'science of synthesis,' we seek to advance and refine the SReP methodology through collaborative exploration and innovation.

Expected Research Achievements

● Innovative Breakthroughs through Strategic Cross-Disciplinary Collaboration

This research initiative comprises three specialized groups, A01 to A03, each focusing on distinct target substances, alongside the Physical Chemistry Group (A04), which provides analytical and simulation bases for Structural Re-Programming (SReP). The realization of SReP is achievable only through the collaborative efforts of these groups. The following sections provide an overview of the individual research contributions of each group and their collaborative endeavors.

A01 (Organic G): The group focuses on SReP for organic molecules, based on three core technologies: breaking strong chemical bonds, editing ring frameworks, and manipulating stereochemistry. These efforts also benefit SReP in inorganic (A02) and macromolecules (A03).

A02 (Inorganic G): Tasked with advancing SReP for inorganic materials, the group addresses precise control and post-editing challenges. The resulting unique inorganic materials will be used as catalysts for SReP in organic (A01) and macromolecules (A03).

A03 (Macromol G): Specializing in SReP across diverse macro-molecules, such as bio/ synthetic polymers and supramolecules, the group develops entities with unique molecular recognition abilities, which will serve as distinctive reaction sites for targets in A01/A02.

A04 (PhysChem G): This group collaborates with A01-A03 through advanced measurement, analysis, and simulation, thereby ensuring comprehensive insights into SReP mechanisms.

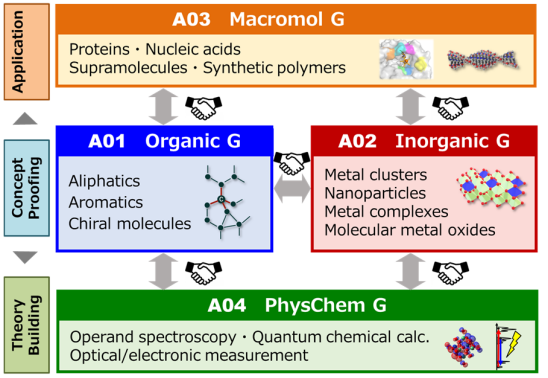

Figure 2. Strategic collaboration

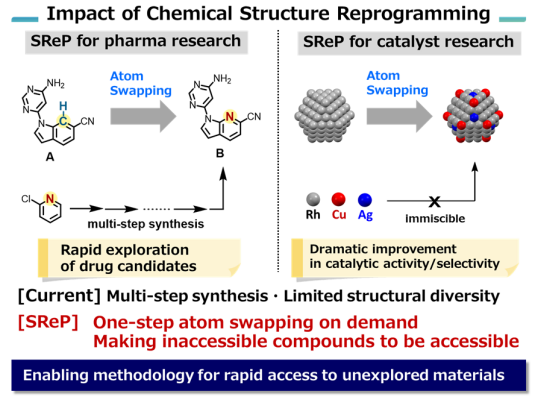

Figure 3. Anticipated applications

● What Benefits Does SReP Offer?

In drug discovery, atom swapping (ex. compound A to B in Fig. 3) often requires intricate, multi-step reactions. Simplifying this process to a single step promises efficient optimization and the discovery of novel candidates. Moreover, once SReP for inorganic materials is established, a diverse range of previously challenging-to-make substances can be synthesized. This advancement facilitates the development of more effective catalysts with refined selectivities. Through pioneering technologies for breaking chemical bonds and arranging atoms precisely, SReP offers rapid access to structural diversity and the production of formerly inaccessible compounds.

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